

Model Performance

Model

Data

Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

**Predicted value:** 186 °C

**Global applicability domain:** Inside

**Local applicability domain index:** 5.26e-01

**Confidence level:** 7.75e-01

Nearest Neighbors from the Training Set

Image not found

Glucovanillin

**Measured:** 189

**Predicted:** 186